WHAT IS CLAIMED IS:

1. A method of identifying a compound which modulates activity of a target RNA comprising

identifying at least one molecular interaction site on said target RNA generating *in silico* a virtual library of compounds predicted or calculated to interact with said molecular interaction site; and

comparing three dimensional representations of said target RNA with members of the virtual library of compounds to generate a hierarchy of said compounds ranked in accordance with their respective ability to form physical interactions with said molecular interaction site.

- 2. The method of claim 1 further comprising synthesizing the highly ranked members of said hierarchy of compounds.
- 3. The method of claim 2 further comprising testing said highly ranked members to determine their ability to interact with said molecular interaction site.
- 4. The method of claim 2 further comprising contacting the target RNA with at least one of said highly ranked members to provide a complex between the RNA and the member or members;

ionizing said complex;

fragmenting the ionized complex; and

determining whether highly ranked members binds to the molecular interaction site of said RNA.

- 5. The method of claim 4 further comprising determining the strength of binding of a highly ranked member in comparison to the binding strength of other highly ranked members,
- 6. A method of identifying a compound which modulates activity of a target biolmolecule comprising

identifying at least one molecular interaction site on said target biomolecule:

generating *in silico* a virtual library of compounds predicted or calculated to interact with said molecular interaction site; and



comparing three dimensional representations of said target biomolecule with members of the virtual library of compounds to generate a hierarchy of said compounds ranked in accordance with their respective ability to form physical interactions with said molecular interaction site.

- 7. The method of claim 6 further comprising synthesizing the highly ranked members of said hierarchy of compounds.
- 8. The method of claim 7 further comprising testing said highly ranked members to determine their ability to interact with said molecular interaction site.
- 9. The method of claim 7 further comprising contacting the target biomolecule with at least one of said highly ranked members to provide a complex between the RNA and the member or members;

ionizing said complex;

fragmenting the ionized complex; and

determining whether highly ranked members binds to the molecular interaction site of said biomolecule.

- 10. The method of claim 9 further comprising determining the strength of binding of a highly ranked member in comparison to the binding strength of other highly ranked members.
- 11. A compound identified in accordance with claim 1.
- 12. A method of modulating the action of an RNA comprising contacting said RNA with a compound identified in accordance with claim 1.
- A pharmaceutical, agricultural chemical or industrial chemical comprising a compound identified in accordance with claim 1.
- 14. A compound identified in accordance with claim 6.
- 15. A method of modulating the action of a biomolecule comprising contacting said RNA with a compound identified in accordance with claim 6.
- 16. A pharmaceutical, agricultural chemical or industrial chemical comprising a compound identified in accordance with claim 6.
- 17. A method of identifying a compound which modulates activity of a parget RNA comprising



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generating *in silico* a virtual library of compounds predicted or calculated to interact with said RNA;

comparing three dimensional representations of said target RNA with members of the virtual library of compounds to generate a hierarchy of said compounds ranked in accordance with their respective ability to form physical interactions with said molecular interaction site; and

synthesizing the highly ranked members of said hierarchy of compounds.

- 18. The method of claim **W** further comprising testing said highly ranked members to determine their ability to interact with said molecular interaction site.
- 19. The method of claim 18 further comprising contacting the target RNA with at least one of said highly ranked members to provide a complex between the RNA and the member or members;

ionizing said complex;

fragmenting the ionized complex; and

determining whether highly ranked members binds to the molecular interaction site of said RNA.

20. The method of claim 19 further comprising determining the strength of binding of a highly ranked member in comparison to the binding strength of other highly ranked members.

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